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Photon and Electron Data for Use in Accelerator Applications

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Abstract

In accelerator applications we need photon and electron data, as well as computer codes that utilize this data, in order to predict results inexpensively and safely. In this paper I will first cover the current status of available photon and electron data, with emphasize on the improved detailed that has only recently been added to our data bases. Next I will cover the availability of this data and computer codes that use it.

Introduction

In the last few years our photon and electron data bases have been greatly improved in terms of the detail included as well as the accuracy of the data. At the same time there has been an enormous increase in our available inexpensive computer power. The combination of improved photon and electron data bases and increased available inexpensive computer power allows us today to calculate results in greater detail, with greater accuracy, using accurate methods, such as Monte Carlo, which was not practical just a few short years ago.

In this paper I will describe the current status of everything that we need in order to perform photon and electron radiation transport calculations. First I will cover the current status of available photon and electron data, with emphasize on the improved detailed that has only recently been added to our data bases. Next I will cover the availability of this data and computer codes that use it.

Photon and Electron Data Bases

I will be discussing three different data bases,

1) the Evaluated Photon Data Library, '97 Version (EPDL97) (ref. 1)
2) the Evaluated Electron Data Library (EEDL) (ref. 2)
3) the Evaluated Atomic data Library (EADL) (ref. 3)

The Evaluated Photon Data Library (EPDL97) describes the interaction of photons with matter as well as the direct production of secondary photons and electron. The Evaluated Electron Data Library (EEDL) describes the interaction of electrons with matter as well as the direct production of secondary electrons and photons. The Evaluated Atomic Data Library (EADL) describes the relaxation of atoms back to neutrality following an ionizing event, i.e., it describes the spectra of radiative (fluorescence) and non-radiative (electron) emitted by an ionized atom as it returns to neutrality.

These three libraries are designed to be used in combination to perform detailed coupled electron-photon radiation transport calculations. They all contain elemental data for Z = 1 through 100, over the energy range 10 eV to 100 GeV. They are all completely consistent with one another in terms of all using the same atomic parameters (e.g., subshell binding energies). These libraries include details that were not previously available to us, or not considered when performing calculations using what I will call traditional photon interaction data.

Traditional Photon Interaction Data

Traditionally the data included in a photon interaction data base has been sufficient to describe the interaction of primary photons with matter. The data traditionally contained in this data base included,

1) Cross Sections: for coherent and incoherent scattering, pair production and photoelectric absorption.

2) Form factors and scattering functions, used to describe the angular distribution of coherent and incoherent scattered photons

Although this data is sufficient to describe the interaction of primary photons, it is not adequate to uniquely define the emission of secondary photons following photoelectric effects, e.g., fluorescence. This data also did not include the effect of anomalous scattering, which significantly effects coherent scattering near and below the photoelectric absorption edges. Lastly this data did not differentiate between pair and triplet production.

Additional Photon Interaction Data

In addition to the data traditionally included, the EPDL97 data base now contains,

1) Cross Sections: for each photoelectric subshell, pair and triplet production cross sections, a coherent cross sections accounting for anomalous scattering.

2) Anomalous scattering factors: used in combination with form factors to describe the angular distribution of coherently scattered photons.

To illustrate the increased detail that this library includes figure 1 shows the traditional lead photon cross sections: essentially we need merely four types of cross sections to describe coherent and incoherent scattering, photoelectric absorption and pair production. Figure 2 illustrates the lead photoelectric subshell cross sections included in the EPDL97 library. Figure 3 illustrates the lead electron ionization subshell cross sections included in the EEDL library. Is it important to have this additional detail?

Traditionally when a photoelectric event occurs all of the energy is assumed to be deposited at the point of the event. Figure 4 illustrates that in fact when a photon undergoes photoelectric absorption just above the K edge in lead, 87.9 % of the energy is re-emitted as fluorescence x-rays just below the K edge, where the cross section is quite small, allowing these x-rays to be quite penetrating. Without photoelectric subshell cross sections it is not possible to accurately define the probability of this fluorescence x-ray emission. Therefore having this detail is indeed important.

Is anomalous scattering important. From figure 1 we can see that with anomalous scattering included the coherent scattering cross section at low energy is decreasing and near 10 eV in lead it is about 10 barns. In contrast, without including anomalous scattering it is about 4480 barns - a factor, not per-cent, an actual factor of 448 times too large. Only if you consider the difference between 10 and 4480 barns to be insignificant would you conclude that this is not an important effect.

Related Data Bases

EPDL97 is designed to be used with two of our other data bases to allow coupled photon-electron transport calculations in order to completely account for the emission of all secondary photons, as well as a more detailed description of energy, dose, etc. deposition within media. These two data bases include: 1) an electron interaction data base, covering the same range of elements (Z = 1 to 100) and energy range (10 eV to 100 GeV) as our photon interaction data base; 2) an atomic relaxation data base, to describe the relaxation of atoms back to neutrality following any ionizing event; during the relaxation, photons (fluorescence) and electrons can be emitted by the atom, which should be considered in a photon-electron calculation, or even in a basic photon transport calculation. Figure 4 illustrates the lead electron ionization subshell cross sections contained in our electron interaction library. Figure 3 illustrates the radiative and non-radiative emission due to a vacancy in the K shell of lead: these results were calculated using our atomic relaxation data base EADL.

What's Missing

We have come a long way in the last few years toward being able to accurately model the transport of photons and electrons through matter, but we still aren't where we would like to be. For complete details of how our data bases could be improved see the EPDL97 documentation (ref. 1). Here I will mention only one thing that is still missing from our data bases, namely photonuclear data. Photonuclear reactions have some potentially very positive effects that we could utilize in our applications, e.g., they can cause strong, very localized energy deposition. They also have some potentially very negative effects, such as activating your accelerator. Suffice it to say that there are a wide variety of reasons why it would be desirable for us to have an accurate generally available data base for photonuclear reactions.

There are a number of currently available radiation transport codes that have internal models that they use to describe photonuclear reactions. However, as yet this data has not been systematically reduced to simple data bases for general use. Currently there is an effort under way to develop a data base of photonuclear reactions and hopefully in the next few years this data will be generally available.

Monte Carlo Radiation Transport

It is very nice that we have these data bases, but without computer codes that actually use them in applications these data bases aren't of much practical use to us. There are lots of available radiation transport codes. Here I will only discuss the one that I am most familiar with - namely TART (ref.4).

Usually when Monte Carlo radiation transport is described it is said that its big advantage is that it can be used to model arbitrary geometry, which is indeed true. However, what it often overlooked is its ability to also accurately model reaction kinematics, something that deterministic methods, such as Sn, have trouble doing. For example, the angular distributions for scattered photons and electrons is extremely anisotropic, which makes it very difficult to accurately model using deterministic methods. In contrast this is no problem at all to accomplish using Monte Carlo, including complete correlation between scattering angle and secondary energy on a continuous basis.

In the past the main reason that Monte Carlo radiation transport was not used more often was that it was considered to be prohibitive expense and not practical if we wish to obtain an accurate answer in a reasonable period of time. It wasn't too long ago that we thought of Monte Carlo radiation transport calculations as limited to a few thousands of particle histories, e.g., track a few thousand photons. This is no longer the case. In just the last few years the tremendous increase in inexpensive available computer power has allowed us to go from thousands, to millions, to billions of histories. For example, today a relatively inexpensive $3,000 PC can be used with TART (ref. 4) to process several billion photon histories per day; something we would have never even thought possible just a few short years ago. If you are a high roller with more computer resources you can push things even further. For example, with today's multi-processor computers that have thousands of processors, you can use TART to process over a trillion (that's right, a trillion, ten to the twelfth power) histories per day.

The bottom line is that it is now practical to efficiently and quickly use Monte Carlo radiation transport to obtain very detailed and accurate answer. With the number of histories that we can now process results have little, if any, statistical uncertainty. In addition Monte Carlo is the only method available to us that can accurately model the increased detail in our currently available data bases, e.g., exact correlated kinematics.

Conclusions

In this paper I have described details of the EPDL97 photon interaction data base. This data base is designed to meet the needs of two different groups of users: 1) Those who would like to use this data in the traditional sense, without including additional details in the calculations - we have taken care to insure that this can still be done, and 2) Those who would like to extend their calculations to include more details in their photon (and if desired, coupled electron) transport calculations. Care has been taken to insure that EPDL97 can be used by either group of users.

The three data bases, EPDL97, EEDL, and EADL are documented in ref. 1, 2 and 3, and TART is documented in ref. 4. All are currently available from data centers throughout the world. To obtain copies of documentation and for details of how to obtain these data bases and/or the TART Monte Carlo radiation transport code see my website at **http://reddog1.llnl.gov**.

References

1) "EPDL97: the Evaluated Photon Data Library, '97 Version," UCRL-50400, Vol. 6, Rev. 5, Lawrence Livermore National Laboratory, Livermore, CA, (September 1997), by Dermott E. Cullen, John H. Hubbell, and Lynn Kissel

2) "Tables and Graphs of Electron-Interaction Cross Sections from 10 eV to 100 GeV Derived from the LLNL Evaluated Electron Data Library (EEDL), Z = 1-100," UCRL-50400, Vol. 31, Lawrence Livermore National Laboratory, Livermore, CA, (November 1991), by S. T. Perkins, D. E. Cullen and S. M. Seltzer.

3) "Tables and Graphs of Atomic Subshell and Relaxation Data Derived from the LLNL Evaluated Atomic Data Library (EADL), Z = 1-100," UCRL-50400, Vol. 30, Lawrence Livermore National Laboratory, Livermore, CA, (October 1991), by S. T. Perkins, et.al

4) "TART97: A Coupled Neutron-Photon 3-D, Combinatorial Geometry Monte Carlo Transport Code, UCRL-ID-126455, Rev. 1, Lawrence Livermore National Laboratory, Livermore, CA, (November 1997), by Dermott E. Cullen

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Figure 1: Lead Photon Interaction
Cross Sections

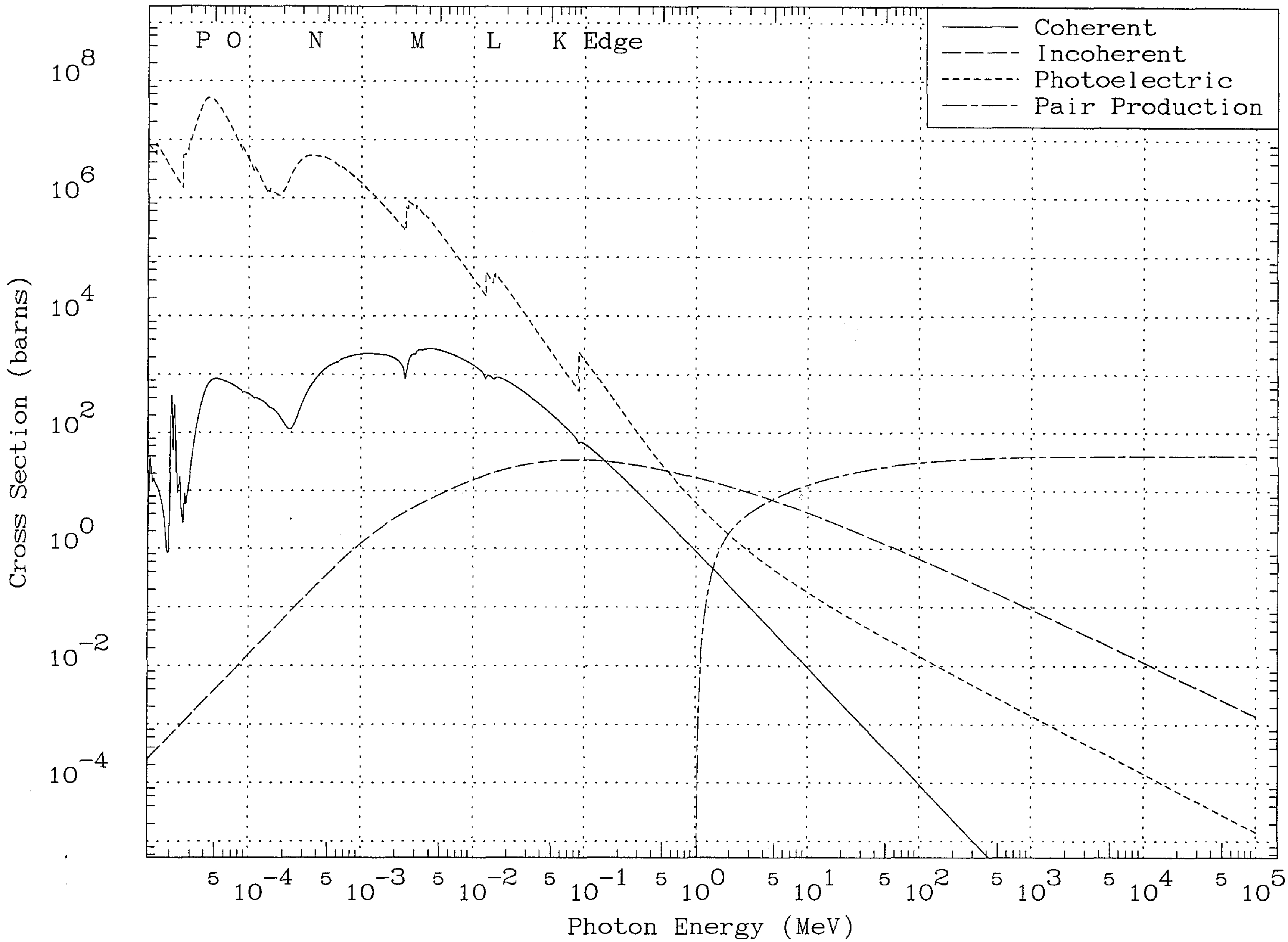

Figure 2: Lead Photoelectric
Cross Sections

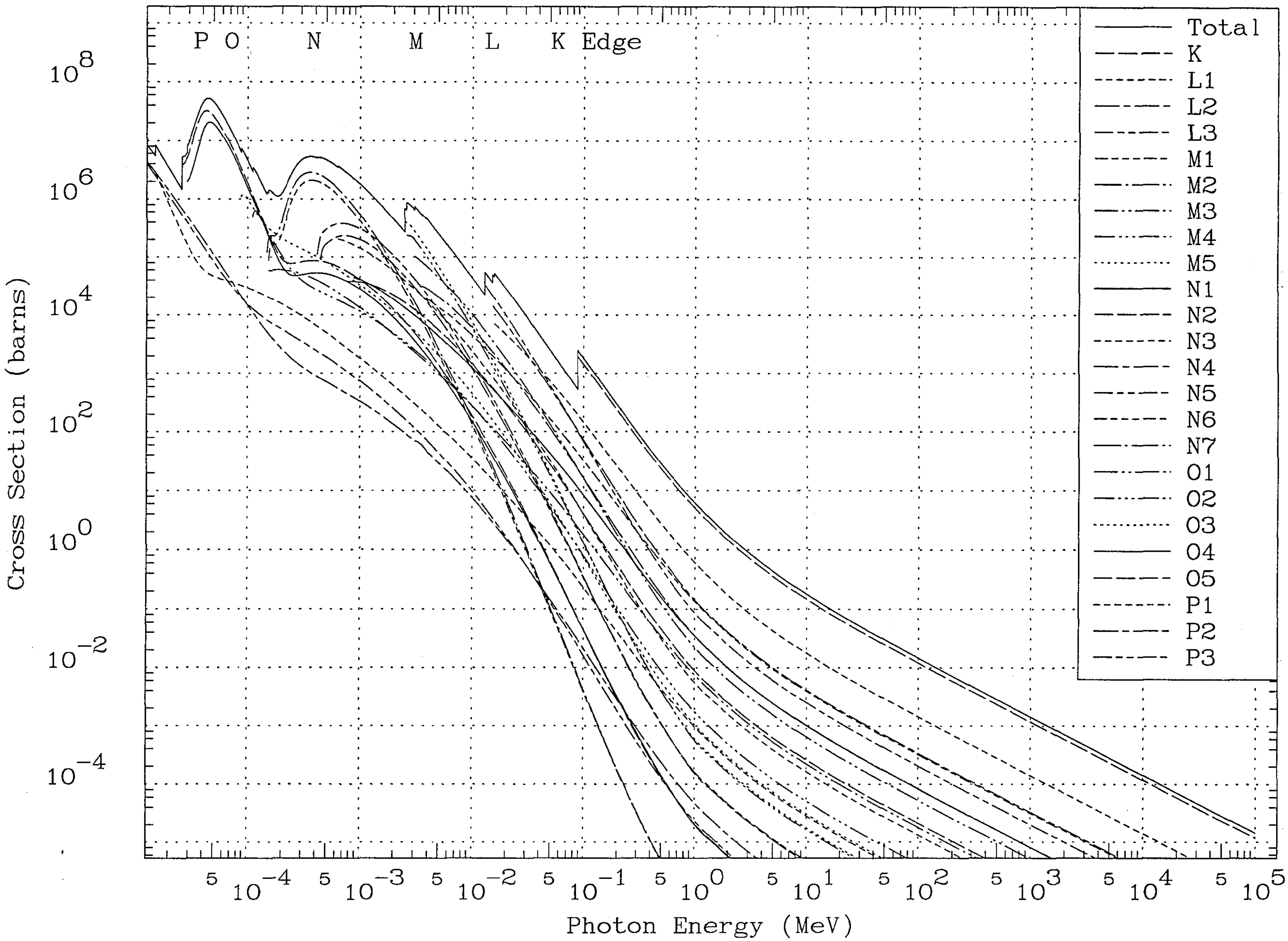

Figure 3: Lead Electron Ionization Cross Sections

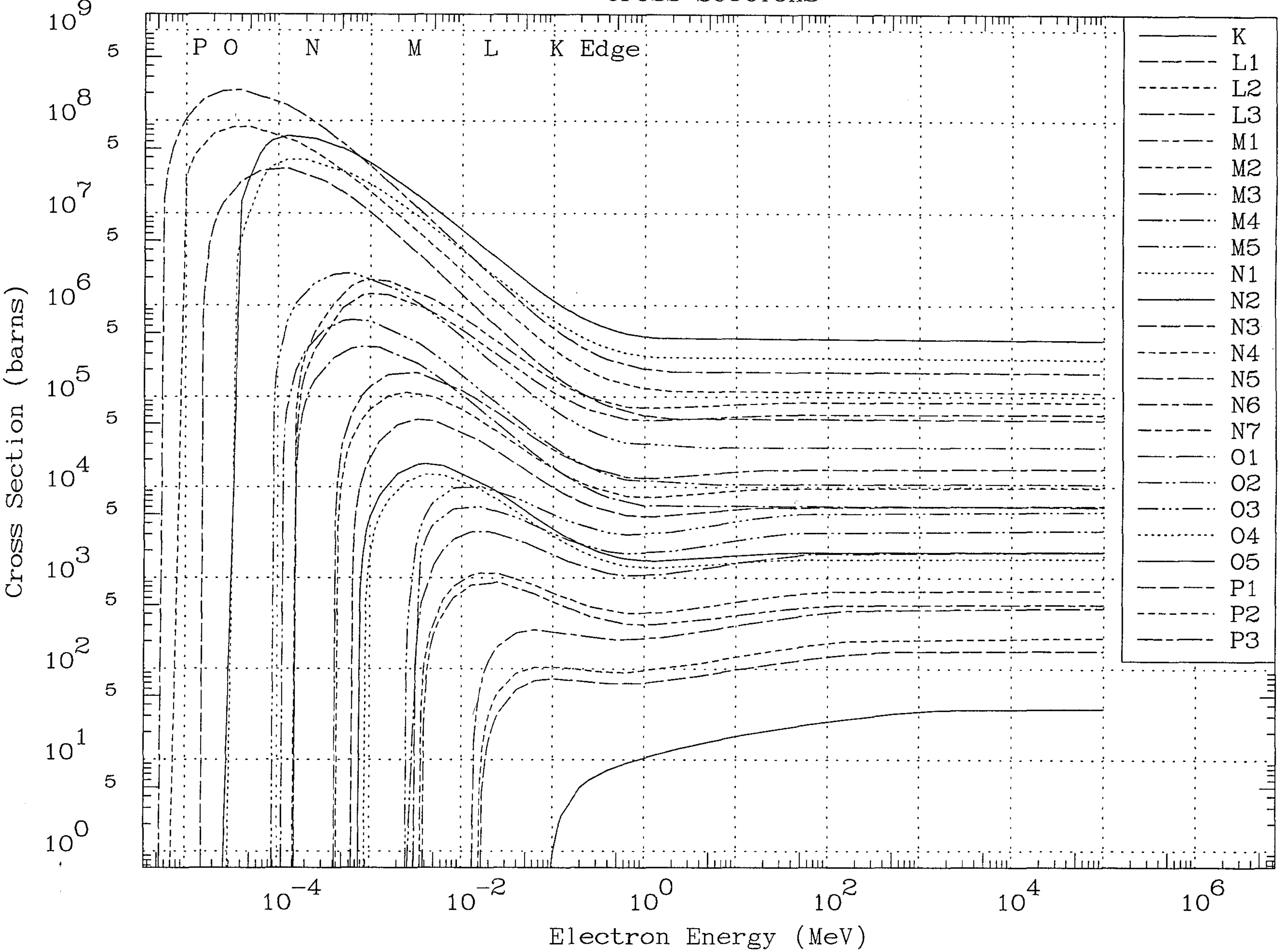

Figure 4: Lead K Shell X-Ray (Fluorescence) Emission
88.3 keV Binding energy